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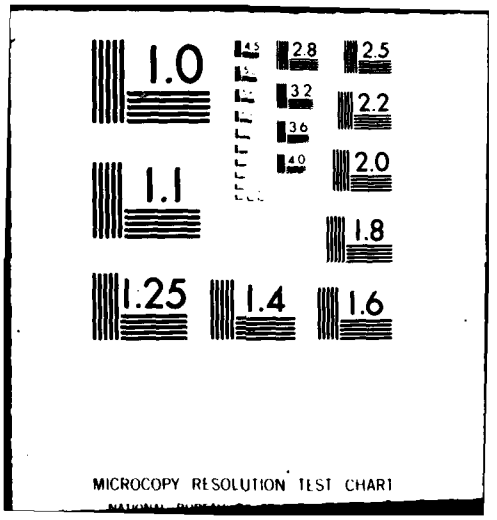
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PHASE DIAGRAM OF ISING MODELS WITH RANDOM SUBLATTICE VACANCIES

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Abstract

We use a modified Kadanoff's variational method to calculate the phase diagram of an Ising model with random vacancies on one of two interpenetrating sublattices of the isotropic square (SQ) and body-centered cubic (BCC) lattices. We find second order phase transitions only for T>0. The transition temperature to very good approximation decreases linearly with impurity (i.e. vacancy) concentration at small concentration. This agrees with the linear decrease observed in other systems. A plausible explanation of the absence of first order transitions for T>0 is given.

The relation of our models to certain percolation problems is similar to that of some spin models studied by Syozi. Thus our results allow an estimate of critical probabilities for percolation.

1. Introduction

In recent years, much attention has been paid to extensions of the ordinary spin 1/2 Ising model, such as the Potts model [1-3] and spin one models [4-11]. An example of the latter is the Blume-Capel model [4,5] represented by the Hamiltonian:

$$H = -J\sum_{<nn>} S_i S_j - D\sum_i (1-S_i^2) - B\sum_i S_i \qquad (1)$$

where s_i, s_j = 1, 0, -1, $\sum_{<nn>}$ is a sum over nearest neighbor s_i, s_j on the lattice, and D is the zero-field splitting parameter. Eq. (1) may be considered as an Ising

model with annealed impurities (or random vacancies) represented by the zero component of spins s_i. The thermal average impurity concentration is controlled by the parameter D. As $D/J \to -\infty$, the system reduces to the pure Ising model. Mean field [5-6], Monte-Carlo[8], and renormalization group [9-11] (R G) studies of Eq. (1) indicate that the order-disorder phase transitions of this model consist of a line which is first order at low temperatures and second order at high temperatures. It is generally agreed that two regions meet at a tricritical point; however, the location of this point is not exactly known.

In this paper, we apply a modified Kadanoff's Variational method (MKVM)[12-15] to calculate the phase diagram of a related model given by:

$$H = -J\Sigma_{<nn>}\sigma_i s_j - D\Sigma_j (1-s_j^2) - B\Sigma_i \sigma_i - B\Sigma_j s_j, \qquad (2)$$

where $\sigma_i = \pm 1$, $s_j = 1, 0, -1$, <nn> denotes nearest neighbors as in Eq. (11), J>0 and D is a zero-field splitting parameter for s_j. We consider Eq. (2) for SQ and BCC lattices in two and three dimensions respectively. We give results for the B=0 case only. The spins s_j are located on one of two interpenetrating sublattices, the spins σ_i on the other. The two dimensional case is illustrated in Fig. 1. In three dimensions the spins σ_i sit on a simple cubic lattice with a spin s_i at the center of each unit cell. Eq (2) may be considered as an Ising model with annealed impurities or vacancies present on any site j of one sublattice when $s_j = 0$. The thermal average of impurities is controlled by D as in Eq. (- D/J→-∞, Eq (2) also reduces to a pure Ising model. In sect. II, we calculate phase diagrams of our model and find that the order-disorder transitions of Eq (2) for T>0 consist of a line of second order transitions only. The first order line found in the phase boundary calculated from Eq. (1) is no longer present. A plausible argument for this difference is given . In sect. III, we consider our models at T→0. Our models are closely related to some systems studied by Syozi[16]. Each of these spin models has a corresponding percolation problem. The spin system phase boundary for the order-disorder transition at T→0 gives an accurate estimate of the critical probability for the corresponding percolation problem. Thus, the critical percolation

probabilities for our models may be estimated from our calculated phase boundaries at T→0.

II. Method of Calculation and Results

The method of calculation is essentially the same as that reported in previous papers [13-14]. We briefly review it here. We consider Eq (2) for two dimensional square (SQ) and three dimensional body-centered cubic (BCC) lattices. The Hamiltonian of Eq (2) may be rewritten as:

$$H = -\sum_R V_R, \tag{3}$$

$$V_R = JS_R(\sigma_1 + \ldots + \sigma_z) + D(1 - S_R^2) + \frac{B}{z}(\sigma_1 + \ldots + \sigma_z) + BS_R, \tag{4}$$

where R is a unit hypercube of the σ spin lattice with z (=2^d, d being the space dimension) σ spins at the corners and one s spin in the center. This is illustrated in Fig. 1 for the two dimensional case. Performing an exact decimation calculation for the partition function of Eq. (3), which sums over the central s spin in each cell, we obtain an effective Hamiltonian for the remaining σ spins. The resulting unit cell potential is:

$$V_{eff} = \beta B(\sigma_1 + \ldots + \sigma_z)/z + \beta D + \ln\{1 + 2\exp(-\beta D)\cosh(\beta B + \beta J(\sigma_1 + \ldots + \sigma_z)\}, \tag{5}$$

where $\beta = \frac{1}{kT}$. In two dimensions, for the case B = 0, which we examine below, Eq (5) is equivalent to a σ spin Hamiltonian with nearest neighbor, next nearest neighbor, and four spins (around a unit hypercube) interactions. In three dimensions, there are also six and eight spin interactions. For given J, D and β, we then use Eq (5) as $\tilde{V}_0$, the initial cell potential, and carry out the step by step RG transformation. We calculate the free energy (f), internal energy (U) and spontaneous magnetization (M) per spin (here $M \propto \langle\sigma_i\rangle + \langle s_j\rangle$). The average occupation number of the zero component of s spin $\langle n_0\rangle$, ie the concentration of impurities or vacancies, is given by:

$$\langle n_0\rangle = -\frac{\partial f}{\partial(\beta D)} = \frac{1}{2}\langle 1 - s_j^2\rangle \tag{6}$$

$\langle n_o \rangle$ is calculated using the chain rule, by the same method used to calculate U and M (Eq (17) of paper 14 with q representing βD). AS $D/J \to -\infty$ or ∞, $\langle n_o \rangle \to 0$ or 0.5 respectively. From the behavior of the coupling constants (tending to larger or smaller values), we know whether the system is in an ordered or disordered state. From a simple ground state energy argument, it is obvious that for B = 0 the order-disorder transitions occur only in the region $\frac{D}{JZ} \leq 1$. The MKVM [14-15] is known to give accurate values for the transition temperature over a wide range of parameter values.

The calculated phase diagrams (for B = 0) are shown in Fig. 2, where T_o is the transition temperature of the pure Ising model calculated with the MKVM method, which gives $\frac{J}{kT_o}$ = 0.4576223 and 0.1621341 for the SQ and BCC lattices respectively. For comparison, the exact [17] or series expansion [18] values of $\frac{J}{kT_o}$ for SQ and BCC lattices are 0.44068679... and 0.15740 $\pm$ 0.0003 respectively. The part of the diagram under the curve is in an ordered state and above the curve in a disordered state. We calculated U, M and $\langle n_o \rangle$ near the phase boundary and found that there is no discontinuity across the phase boundary even as $\frac{D}{JZ} \to 1$ and $T_c \to 0$. For example, for SQ lattices at $\frac{D}{JZ}$ = 0.9925, we found that $\Delta U \simeq 10^{-16} J$, $\Delta \langle n_o \rangle \simeq 10^{-13}$ and $\Delta M \simeq 10^{-2}$ where $\Delta Q \equiv Q(T+\epsilon) - Q(T_c-\epsilon)$ with Q being U, $\langle n_o \rangle$ or M, T_c being the phase transition temperature for given $\frac{D}{TZ}$ and ϵ being a very small number. The ΔQ values just mentioned are of the same order of magnitude as numerical errors arising from truncation and the approximate location of T_c, etc. We may thus conclude that the transition is always second order rather than first order for T>0. In Fig. 3, we have converted the phase diagram of Fig. 2 to T_c/T_o versus $\langle n_o \rangle$. It is interesting to note that as $\langle n_o \rangle$ approaches the critical concentration $\langle n_o \rangle_c$, above which there is no phase transition at all, T_c decreases smoothly to zero at $\langle n_o \rangle_c$ = 0.26 in the SQ lattice while T_c jumps rapidly to zero near $\langle n_o \rangle_c$ = 0.42 in the BCC lattice. In the later case U and M still change continuously when crossing the phase boundary. Mean field [6] and Monte-Carlo [8] studies of the phase diagram for the Blume-Capel Model (on a SQ lattice) indicate that at T = 0, $\langle n_o \rangle_c$ for this model is 1.0.

The part of Fig. 3 for small $\langle n_0 \rangle$ is enlarged and reproduced in Fig. 4, which indicates that, to very good approximation, T_c decreases linearly with $\langle n_0 \rangle$ for small $\langle n_0 \rangle$. The slopes of the straight lines in Fig. 4 are 1.683 ± 0.002 and 1.116 ± 0.001 for SQ and BCC lattices, respectively. The phase transition temperatures of the Ising model with quenched [19] or annealed [20] bond impurities have also been studied by series expansion method and are found to decrease linearly with small impurity concentration. It has also been observed experimentally [21] that in nickel-rich, nickel-titanium alloys the ferromagnetic Curic temperature decreases, to very good approximation, linearly with titanium concentration x, for $x \lesssim 1.5\%$. The approximately linear decreast of T_c with small impurity concentration is perhaps a rather general phenomena.

Now, we give a plausible explanation for the absence of a first order phase transition in the model of Eq. (2) for T>0. A system at a second order phase transition is characterized by an infinite correlation length ξ, ie a perturbation at one point can propagate to points an infinite distance away. In the model of Eq. (2), the impurities (zero component of s_j) appear only on one sublattice. In the region of interest, $\frac{D}{JZ} < 1$, the spins σ on the other sublattice always have non-zero effective coupling (see Eq. (5)). Thus the correlation length can easily extend to infinity at T_c, in contrast to the model of Eq. (1), where impurities can appear in both sublattices and thus more easily destroy the propagation of a perturbation from one point to another far away point.

We can also understand the absence of first order transitions as follows. For a square lattice one expects a first order transition for $\frac{D}{4J} \lesssim 1$, at low T values, if it exists anywhere. It follows from Eq. (5) that the (exact) decimation of the spins s_i generates (for B = 0) effective nearest neighbor, next nearest neighbor, and four spin interactions that we denote J_{nn}, J_{nnn}, and J_4 respectively. By permutation symmetry one has $J_{nn} = J_{nnn}$. In general, $J_{nn} > 0$ for ferromagnetic J (J > 0). In the region of possible first order transitions one can show that $J_4 > 0$ as well. Thus when the vacancies are summed away all interactions promote

ferromagnetic ordering of the σ spins in this region, and a second order transition (of simple Ising type) is to be expected, as we find in our MKVM calculation. The conclusion of the absence of first order transitions on a BCC lattice for $\frac{D}{8J} < 1$ can also be reached by a similar argument.

III. Low Temperature Limits

Syozi [16] has calculated the exact phase diagrams of Ising models on decorated square (SQ), honeycomb (HC) and plane triangular (PT) lattices with spins $s = \frac{1}{2}$ on each lattice site and spins $s = 1$ on each nearest neighbor bond. He also calculated phase diagrams for Ising models on a semi-dilute honeycomb lattice where the spins $s = \frac{1}{2}$ and $s = 1$ spins are on two equivalent interpenetrating sublattices as in the present case. The phase boundaries of Syozi's models at $T \to 0$ give the critical concentration P_c of spins ($1-P_c$ is the vacancy concentraiton) on sites of $s = 1$ spins above which ferromagnetism can occur. It turns out that P_c calculated in this way is exactly equal or very close to the critical probability of the corresponding bond [22] (for decorated lattices) or sublattice-site (for semi-dilute HC lattice) percolation problems. For the Syozi model:

$$P_c \text{ (decorated SQ)} = 0.5$$

$$P_c \text{ (decorated PT)} = 1 - P_c \text{ (decorated HC)} = \frac{5(3-\sqrt{3})}{18} = 0.3522 \ldots$$

$$P_c \text{ (semi-dilute HC)} = 0.5.$$

For the percolation problem 22, 23.

$$P_c \text{ (bond, SQ)} = 0.5$$

$$P_c \text{ (bond, PT)} = 1 - P_c \text{ (bond, HC)} = 2 \sin \frac{\pi}{18} = 0.349\ldots$$

$$P_c \text{ (sublattice site, HC)} = 0.5 \qquad (8)$$

It is obvious that our model of Eq (2) on the SQ and BCC lattices is just an Ising model on a semi-dilute SQ or BCC lattice and its low temperature behavior is similar to the Syozi models. Thus, the critical probabilities P_c of the sublattice-site percolation problem on the SQ and BCC lattices can be estimated from $\langle n_0 \rangle_c$ of Fig. 3. P_c is given by :

$$P_c = 1 - 2 \langle n_0 \rangle_c. \qquad (9)$$

Applying Eq. (9) to $\langle n_0 \rangle_c$ of Fig. 3, we have P_c = 0.48, 0.16 for the SQ and BCC lattices respectively.

Acknowledgments

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Figure Captions

Fig. 1. Lattice of Eq. (2) in two dimensions. Dots (.) spins σ_i, crosses (x) spins s_j. The dotted lines enclose a unit hypercube of the σ spin lattice.

Fig. 2. Transition temperature T_c vs. D/Jz obtained for a two dimensional SQ (+) lattice and a three dimensional BCC (Δ) lattice.

Fig. 3. Transition temperature vs. impurity concentration $\langle n_o \rangle$ for a SQ (+) and a BCC (Δ) lattice.

Fig. 4. Part of the curves in Fig. 3 for $\langle n_o \rangle$ <2.6%. The solid curves are obtained by a linear least square fit to the data points.

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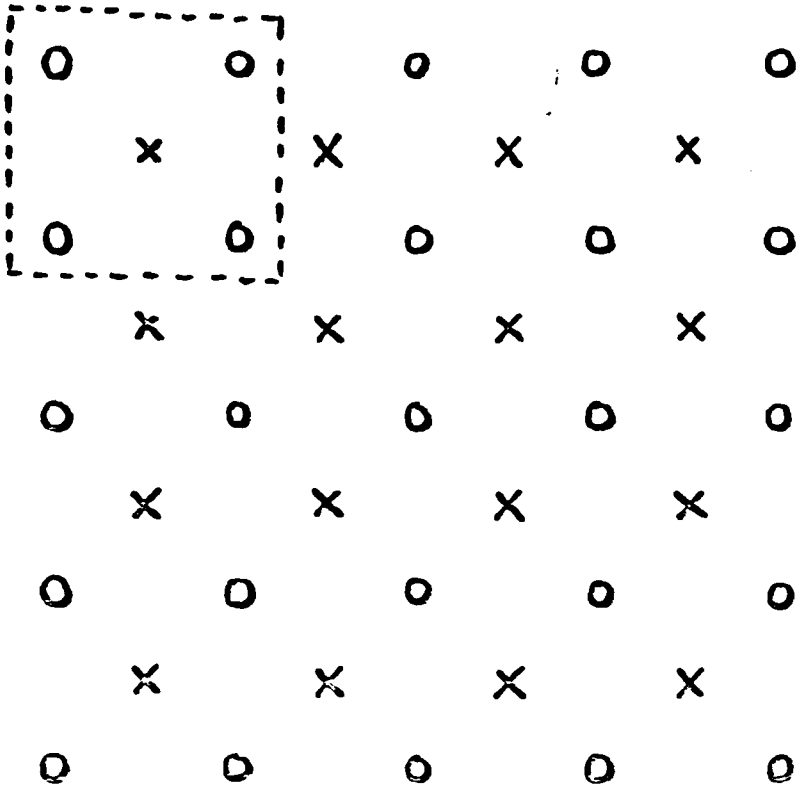
23. In the sublattice-site percolation problem, the sites on one of two equivalent sublattices are occupied completely by atoms (ie with probability 1), the sites of the other sublattice are occupied with probability P. The sublattice-site percolation problem on a honeycomb lattice is equivalent to the site percolation problem on a triangular lattice whose critical probability is 0.5.



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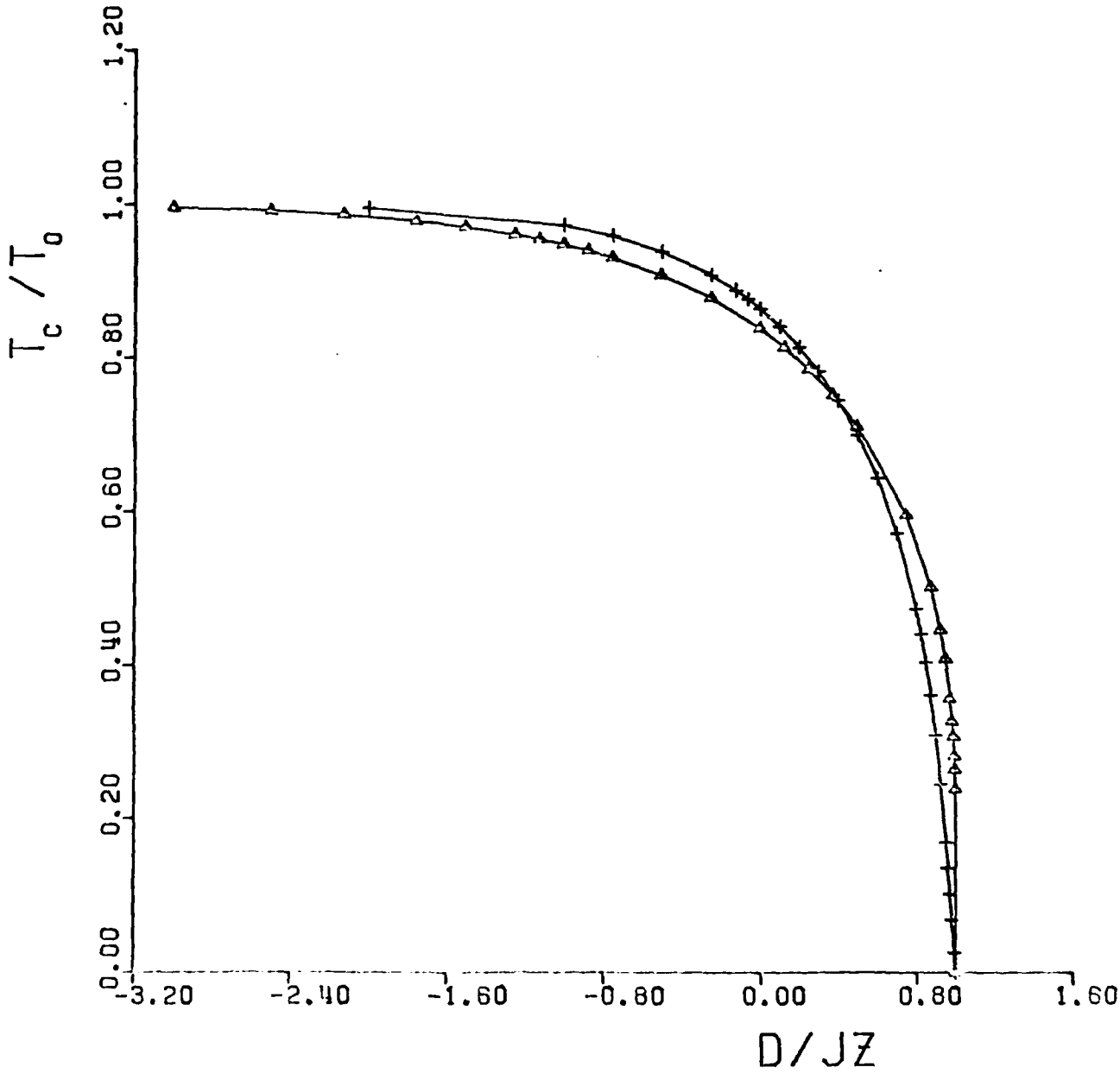

Fig 2

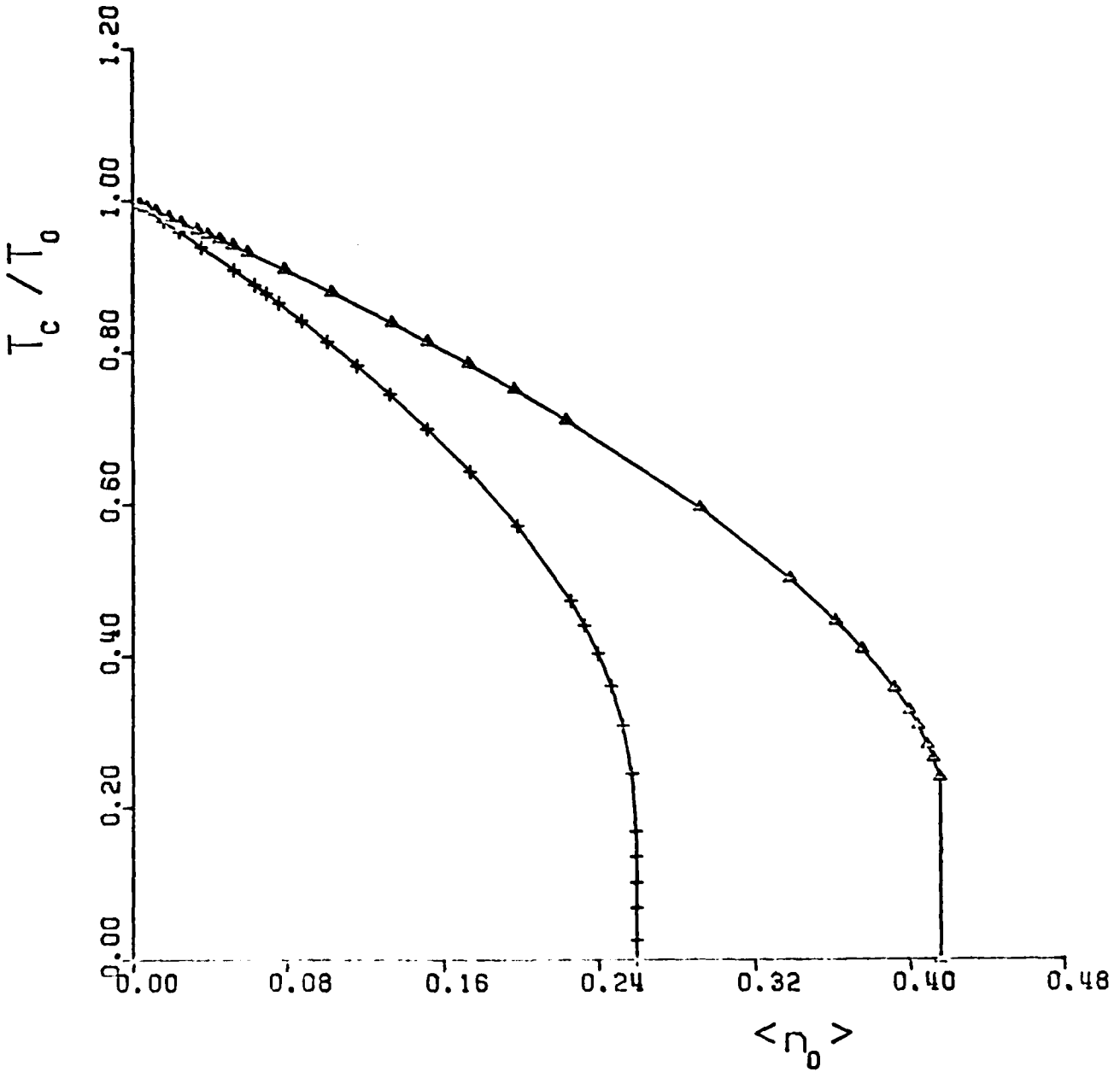
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Fig 3

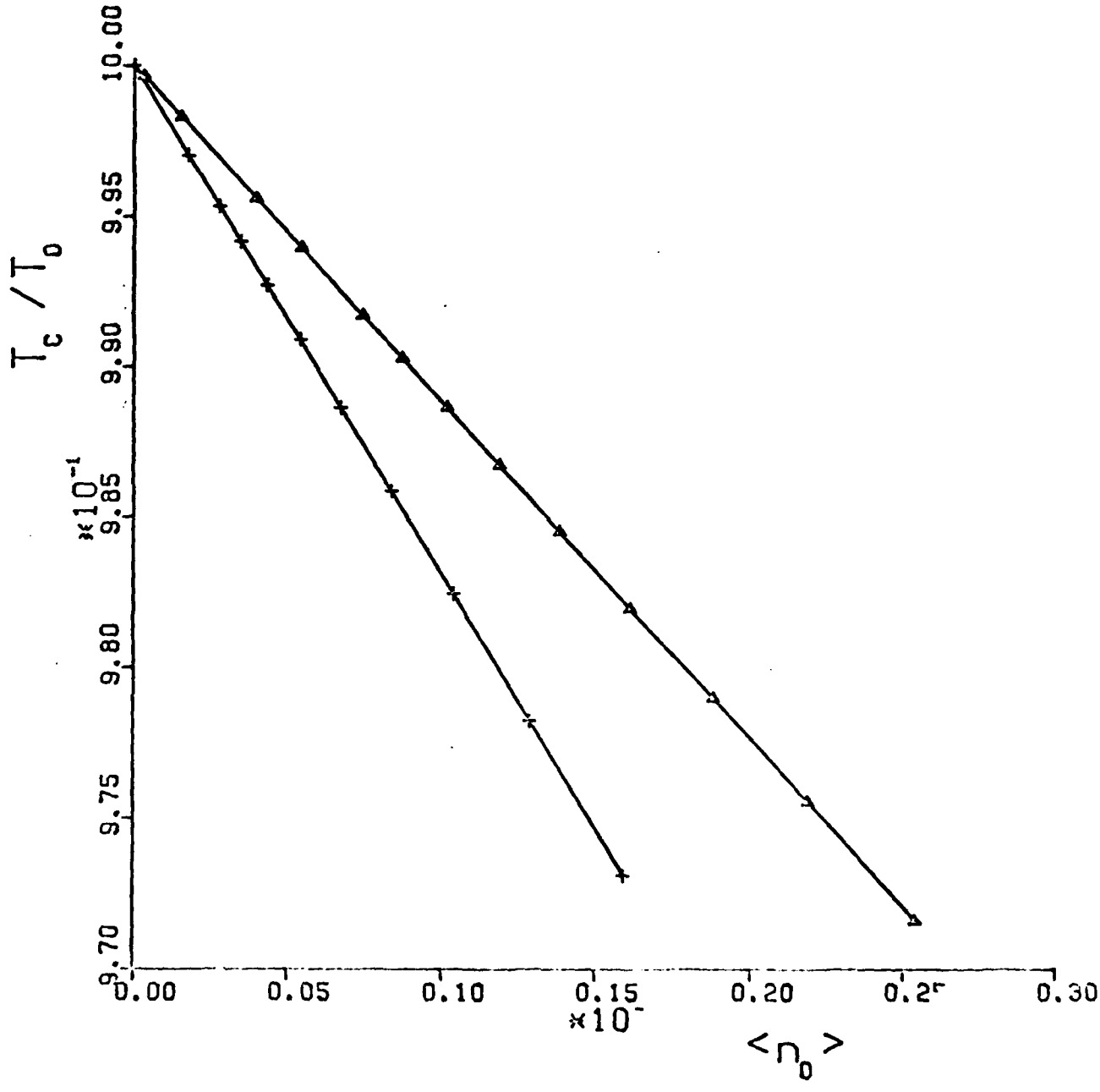
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Fig 4


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